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Marine reptiles flourished in the Mesozoic oceans, filling ecological roles today dominated by crocodylians, large fish, sharks, and cetaceans. Many groups of these reptiles coexisted for over 50 million years, through major environmental changes. Little is known, however, about how the structure of their ecosystems or their ecologies changed over millions of years. We use the most common marine reptile fossils—teeth—to establish a quantitative system that assigns species to dietary guilds, and then track the evolution of these guilds over the ca. 18 million year history of a single seaway, the Jurassic Sub-Boreal Seaway of the United Kingdom. Groups did not significantly overlap in guild space, indicating that dietary niche partitioning enabled many species to live together. Although a highly diverse fauna was present throughout the history of the seaway, fish and squid-eaters with piercing teeth declined over time while hard-object and large-prey specialists diversified, in concert with rising sea-levels. High niche partitioning and spatial variation in dietary ecology related to sea depth also characterize modern marine tetrapod faunas, indicating a conserved ecological structure of the world's oceans that has persisted for over 150 million years.

During the Mesozoic Era, when dinosaurs ruled the land, the oceans were teeming with a diversity of large reptiles adapted to an aquatic lifestyle[1-4]. These included iconic groups such as the long-necked plesiosauroids, big-headed pliosaurids, dolphin-like ichthyosaurs, and an aberrant assemblage of crocodile relatives called thalattosuchians (subdivided into the gharial-like teleosaurids and cetacean-like metriorhynchids). These groups were exceptionally diverse and coexisted in the same environments for over 50 million years, from the Early Jurassic (ca. 180 million years ago) to the Early Cretaceous (ca. 130 million years ago)[5-12], through major changes in sea-level, climate, and ocean chemistry. They formed complex ecosystems and filled a variety of ecological roles—ranging from fast-swimming fish-eaters to large-bodied apex predators[7-9]—that are today dominated by crocodylians (in near-shore environments), sharks and other large fishes, and marine mammals[1-2,13]. As modern oceans are undergoing rapid changes, understanding Mesozoic marine reptile ecosystems may provide critical insight into how species at or near the top of the food chain might respond to environmental shifts.

Although the phylogenetic relationships and taxonomic diversity patterns of Mesozoic marine reptiles have been the subject of intensive focus[14-19], much less is known about their ecology, about the structure of their ecosystems, and how their ecosystems changed over millions of years of evolutionary time. Two main problems have hindered progress. First, it is difficult to determine the ecological niches and feeding styles of extinct species, particularly when they are represented by limited fossil material. The pioneering work of Massare[7-8] assigned marine reptiles to broad ecological guilds, but these are qualitative in nature and have not been universally acccepted[9]. Second, the marine reptile fossil record is notoriously patchy, dominated by fossil-rich localities (Lagerstätten) that register snapshots of ecosystems but do not document long-term changes[3]. These issues hamper comparisons

between Mesozoic and modern marine faunas, and make it difficult to draw parallels between the fossil record and contemporary environmental change.

Here, we use teeth—the most common marine reptile fossils, which are often preserved in the absence of more complete skeletal remains—to evaluate feeding ecology. Our quantitative approach validates the guild system of Massare[7-8], and allows species to be placed in a functional morphospace that reflects the breadth of dietary niches. We then track changes in how these niches were filled over time, focusing on the remarkable fossil record of the Jurassic Sub-Boreal Seaway of the United Kingdom. Marine reptiles have long been known from two Lagerstätten formed in this seaway, the Oxford Clay Formation (Callovian-early Oxfordian, ~165-161 Ma) and the Kimmeridge Clay Formation (Kimmeridgian-early Tithonian, ~157-148 Ma)[20-21], but recent work has clarified the fossil record of the intervening Corallian Group (~161.5-157.3 Ma)[17,22]. Thus, we can now examine long-term ecological changes in a single seaway spanning ca. 18 million years of the Middle-Late Jurassic, a time of known environmental changes that began with recovery from a drop in sea-level linked to a major glaciation, followed by a gradual rise in sea-level that culminated in a chaotic interval of rapid shifts in water depth[23-30].

Results

Principal Coordinates Analysis (PCO) of our dental morphology dataset ordinated all specimens into a morphospace, the first three axes of which describe over 63% of total variance (Fig. 1; Supplementary Figures 2-3; Supplementary Table 1). A linear discriminant analysis found that clusters of species in the morphospace correspond to the feeding guilds of Massare[7], originally qualitatively defined based on comparisons of tooth shape, wear, and size and with modern marine tetrapods (Supplementary Table 6). When the 35 specimens in

74 our dataset (encompassing 25 taxa) that were also included in Massare's study were assigned
75 to Massare's guilds *a priori*, a jackknifing procedure found that our PCO axes successfully
76 discriminated these groups, with 84% of species correctly attributed to the guild Massare
77 assigned them to. This supports broad correspondence between our PCO morphospace and
78 Massare's guilds, but 16% of species are mis-attributed, which may be because some species
79 previously known from limited fossil material (particularly metriorhynchids) were
80 misclassified when Massare introduced the guilds. We therefore used our PCO results to
81 establish a revised system of five guilds, which linear discriminant analysis finds to be
82 97.30% accurate. Along with the fact that characters in our dataset were chosen to represent
83 functionally significant features related to feeding, this indicates that the PCO morphospace
84 can be interpreted as a functional morphospace reflecting diet (Table 1). This link was
85 previously demonstrated by Massare[7], by assessing tooth morphology, shape and gut contents
86 of the same species, and validated with comparisons with modern marine tetrapods (for
87 which dietary data are available).
88

Guild		**Apex shape**	**Ornamentation**	**Cutting edges**	**Tooth size and shape**	**Examples**
Cut		Pointed	Normally largely absent (in geosaurines, except cf. *'Metriorhynchus' hastifer*)	Two functional cutting edges always present	Very large: generally > 4cm. Robust crowns, mid-to-high CR*	*Dakosaurus, Plesiosuchus,* ***Geosaurus****,* cf. *'Metriorhynchus' hastifer*
Generalist	**Generalist-Cut**	Pointed	Present: high-relief with serration morphologies	Two or more cutting edges always present	Very large: generally > 5cm. Robust crowns, mid-to-high CR*	*Pliosaurus* spp.
	Generalist-Pierce	Pointed	Variable, it may be high relief	None, or non-prominent. If present they are smooth and non-serrated	Variably large: generally > 5cm. Normally conical. Variable CBR.	***Liopleurodon, Simolestes, 'Pliosaurus' andrewsi***

Pierce	Pointed	Variable, but never high relief	None, or non-prominent. In metriorhynchines if they are present they are smooth, or not functionally serrated.	Normally small (<3cm), but can be large (>3cm). Mid-to-high CR*, lateral compression variable (weak or absent, in plesiosauroids and metriorhynchines; laterally compressed in geosaurines).	All plesiosauroids, **MJML K1885,** *'Steneosaurus' leedsi, Mycterosuchus, Gracilineustes, Peloneustes;* ***Metriorhynchus, Suchodus,*** *Tyrannoneustes, 'M.' cultridens*
Smash	Pointed to Rounded	NA	None	Conical. Mid-CR*	*Ophthalmosaurus,* ***Brachypterygius***
Crunch	Rounded	Strongly ornamented, with high-relief ridges and may have serration morphologies	Prominent carinae only on the top half of the crown.	Robust and conical, poorly to non-laterally compressed. Mid-to-low CR*.	*Lemmysuchus, Machimosaurus, Torvoneustes*

Table 1. Description of the main tooth features diagnosing the five guilds as used in this study. Note that this is a key that can be used to assign specimens to guilds based on consideration of a few general features, but more rigorous assignment can be made numerically using Linear Discriminant Analysis of PCO scores. Taxa in bold are classified in a different guild compared to Massare's System[7] (see Supplementary Table 7, Appendix S3, S4). The table is adjusted from Massare (1987)[7]. *CR: Crown height to base Ratio.

Many thalattosuchians (teleosaurids and metriorhynchids), plesiosauroids, and small-bodied pliosaurids cluster together in morphospace, due to their thin teeth that lack serrations (Pierce Guild), similar to modern shallow-water river dolphins and gharials; they are inferred to be fish and squid-eaters (Fig. 1, Table 1). An adjacent region of morphospace is occupied by the soft prey-eating Smash Guild, which is almost exclusively filled by ichthyosaurs with conical, non-carinated and non-serrated teeth (Fig. 1, Table 1). Strongly ornamented, blunt crowns of machimosaurin teleosaurids and the geosaurine *Torvoneustes* belong to the Crunch Guild, inferred as hard-object (e.g. sea turtles) feeders (durophages) (Fig. 1, Table 1). There are two clusters of cutting-type dentitions that correspond to different types of macrophagy (feeding on large-bodied prey), analogous to modern deep-water cetaceans like killer whales: the Cut Guild of geosaurine metriorhynchids (*Geosaurus*, *Plesiosuchus*, and *Dakosaurus*) with large and serrated teeth, and the Generalist-Cut Sub-Guild (the macrophagous partition

of the Generalist Guild) of pliosaurids with huge, robust, heavily ornamented teeth (*Pliosaurus*) (Fig. 1, Table 1). The Generalist-Pierce Sub-Guild (the other partition of the Generalist Guild), characterised by large, conical and variably ornamented teeth and mostly including large Callovian pliosaurids, fills a space between the Generalist-Cut and Pierce Guilds (Fig. 1, Table 1).

We assessed changes in the dietary ecology of marine reptiles during the ca. 18 million year history of the Sub-Boreal Seaway by testing for changes in morphospace overlap and morphological disparity (amount of occupied morphospace) between phylogenetic groups. The major marine reptile groups do not significantly overlap in morphospace overall, and within each time slice (Appendix S2), indicative of large-scale dietary niche partitioning, but also a likely phylogenetic signal (e.g. through shared evolutionary ancestry). However, individual groups show evidence of morphospace migration over time (Fig. 2). Pliosaurids are the most extreme example, as they make a (nearly) significant jump (Supplementary Table 2) between their scattered Callovian morphospace into a more restricted region in the ensuing Oxfordian. This change is followed by another significant shift between the Oxfordian and Kimmeridgian, as a consequence of the appearance of the genus *Pliosaurus*.

Other groups do not exhibit significant shifts between successive time intervals, but do show significant changes between end points (e.g., Callovian vs. Tithonian, or Oxford Clay vs. Kimmeridge Clay Formations), which is indicative of gradual ecological changes.

There are no significant differences over time in the disparity of the pooled sample of all marine reptile groups in the morphospace (as shown by permutation tests on range and variance measures of morphospace occupation), indicating that an ecologically diverse fauna persisted throughout the entire history of the seaway (Supplementary Table 5). There are few instances of significant disparity changes within individual groups across successive time intervals, despite turnover at the species level (Fig. 2). Metriorhynchid groups are the

exceptions, as geosaurines significantly increased in disparity from the Oxfordian to the Kimmeridgian, as their variety of niches expanded, in concert with the decline of fish-eating metriorhynchines. This implies that, although groups were migrating through morphospace over time, most continued to fill a similar breadth of niches, albeit in different regions of the morphospace (Fig.2). Partial disparity trends show that teleosaurids and metriorhynchids make up a large proportion of overall disparity in the Callovian but decline over time, whereas geosaurines and macrophagous pliosaurids (*Pliosaurus*) become relatively more disparate (Fig. 3). When partial disparity is instead tracked by guild, Pierce taxa are highly disparate early but decline into the Oxfordian and beyond, as Crunch, Smash, and Cut species assume a larger share of overall disparity (Fig. 3).

These quantitative tests allow us to identify several major trends. Pliosaurids were diverse in the Callovian, ranging across a broad span of fish-eating Pierce and apex-predator Generalist/Generalist-Pierce guilds, but then in the Oxfordian atrophied into a more restricted region of macrophagous morphospace (Generalist/Generalist Cut), where they diversified further in the Kimmeridgian, without migrating back into the Pierce Guild. Similarly, teleosaurids were highly diverse in the Callovian, including long-snouted fish-eaters in the Pierce Guild and durophages in the Crunch Guild, but the former species mostly disappeared from the Oxfordian onwards while the hard-object feeders persisted. Geosaurines began with a large diversity of taxa spanning the Pierce Guild in the Callovian, and in the Oxfordian bifurcated into a Crunch group that approached the durophagous teleosaurids in morphospace and a Cut group of large-prey specialists, which were distinct from the macrophagous Generalist-Cut pliosaurids in morphospace. Metriorhynchines included several Pierce Guild piscivores in the Callovian, but then mostly disappeared afterwards. Ichthyosaurs were relatively stable in almost exclusively occupying the soft-prey-eating Smash Guild from the Callovian to Tithonian, but their share of partial disparity increases over time. Sample sizes

for plesiosauroids are too small to reasonably interpret, although they seem to stably occupy the Pierce Guild through time.

Discussion

In agreement with previous studies[5,7,15], we argue that there is a tight link between tooth morphology and dietary ecology in Jurassic marine reptiles. By assessing a limited number of discrete features and measurements of the teeth, species can be placed in a functional morphospace that distinguishes ecological guilds (Fig. 1). This morphospace differentiates marine reptiles that fed in different ways, including soft-object feeders, piercers of fish and squid, durophagous hard-object crushers, and apex predator macrophages that specialized on large vertebrate prey[5,7,15]. Our approach is a powerful tool for predicting the feeding habits of long-extinct species, as it focuses on the most commonly preserved marine reptile fossils (teeth), and can incorporate even minimally complete specimens. Our approach provides a quantitative method for projecting Massare's guilds[7]—which have long been used by marine reptile workers—into a numerically-derived morphospace, meaning specimens can be assigned to these guilds more objectively, and changes in guild occupation over time can be analysed statistically.

Our study reveals the ecological structure of marine reptile faunas in the Sub-Boreal Seaway during ca. 18 million years of the Middle-Late Jurassic. The positions of species in our functional morphospace give insight into niche occupation. The major marine reptile groups do not significantly overlap with each other in morphospace, meaning that different groups generally employed distinct dietary strategies (possibly in part due to shared evolutionary ancestry). Partitioning niches in this way may explain why such a great diversity of marine reptiles were able to coexist in the Mesozoic oceans[13], and parallels the situation in modern oceans, where aquatic tetrapods subdivide ecological space by feeding in different

ways and on different prey[31-40]. Evidently, Jurassic marine reptiles partitioned niches to a fine degree, as testified by the development of two distinct and coexisting forms of macrophagy: the robust-toothed pliosaurids in the Generalist-Cut Guild and the thinner, slicing-toothed geosaurines of the Cut Guild. Other groups converged on similar niches—most notably machimosaurin teleosaurids and *Torvoneustes*-lineage geosaurines that independently colonized the same durophagous area of morphospace—which speaks to the maintenance of key niches over long spans of time. We also find no significant differences in overall morphological disparity of the Sub-Boreal assemblages over time, illustrating that a diverse marine reptile fauna was present throughout the entire history of the seaway, and in general terms was resilient to environmental change.

Nonetheless, the shifting distribution of species in the morphospace over time does provide evidence for long-term ecological changes. Although the imprecise ages of fossils make it difficult to untangle the tempo of these changes, they appear to be a mix of sudden transformations at or near the Callovian-Oxfordian (Middle-Late Jurassic) boundary and more gradual changes that occurred throughout the Oxfordian, Kimmeridgian, and Tithonian, as sea-levels rose and water depth increased. Most severe was the decimation of the Pierce Guild, which was filled by a diversity of teleosaurids, metriorhynchines, and small-bodied pliosaurids in the Callovian, but was then largely vacated from the Oxfordian onwards. Essentially, this reflects a drastic decline of nearshore, piscivorous species. Metriorhynchines excelled in this niche and were the most abundant component of the Callovian Oxford Clay ecosystem, but are almost unknown from the later Kimmeridge Clay. Replacing the Pierce species was a greater variety of macrophagous taxa, particularly large pliosaurids and geosaurines, and durophages, including the specialized machimosaurin lineage of teleosaurids. At the same time, ichthyosaurs maintained their position in the Smash Guild and diversified further, reflecting a blossoming of deep-diving species that fed on similar prey to

206 the more nearshore piercers that were devastated.

207 We hypothesize that these large-scale changes in marine reptile functional diversity
208 and niche occupation in the Jurassic Sub-Boreal Seaway were related to changes in water
209 depth over time, analogous to how modern aquatic tetrapod diversity and ecology are known
210 to change from shallow water (nearshore) to deeper water (offshore) habitats[31-40]. It is well
211 established that the Sub-Boreal Seaway became generally deeper as global sea-levels rose
212 from the Callovian into the Oxfordian, and then across the Oxfordian, Kimmeridgian, and
213 early Tithonian. The main fossiliferous beds of the Callovian Oxford Clay Formation were
214 deposited in nearshore waters ca. 50 metres deep[25-26,30]; the middle-late Oxfordian Corallian
215 Group rocks formed in deeper waters during a time of warming and sea-level
216 transgression[17,20-22,27-28,30]; and the main fossil-bearing units of the Kimmeridge Clay
217 Formation, spanning the Kimmeridgian-Tithonian boundary, were deposited on continental
218 shelves 100-200 metres deep[29,30]. Although numerous factors (ranging from water
219 temperature and turbidity to productivity and seasonality) control the distribution of extant
220 marine tetrapods and their prey, water depth is widely recognized as one of the key drivers of
221 ecological partitioning[33-40]. While small delphinoids such as bottlenose and spotted dolphins
222 can be found both nearshore and sometimes further shelf-ward, large delphinoids like killer
223 whales predominately live in deeper, open waters and infrequently venture nearshore[36-38], and
224 their abundance on continental shelves increases with water depth[39]. The diets of mid-shelf to
225 offshore delphinoids also becomes increasingly dominated by larger prey, and only off-shelf
226 species actively prey upon large tetrapods[13,31,39].

227 In the Jurassic Sub-Boreal Seaway, a variety of marine reptiles shared environments
228 by feeding in different ways, and nearshore fish-eating marine reptiles declined and open-
229 ocean macrophages and durophages proliferated as sea-level increased over millions of years
230 of evolutionary time. In the modern oceans, numerous species of large vertebrates coexist by

partitioning dietary niches, and there is a noted ecological partitioning of shallow-water small-object feeders and deep-water, large-prey specialists. These parallels between Jurassic and modern oceans—separated in time by ca. 150 million years, occupied by different groups of species, and shaped by vastly distinct paleogeography, temperature, and ocean chemistry—may indicate a conserved ecological structure near the top of ocean food webs over time.

Methods

Dataset. We compiled a dataset of 22 functionally-relevant anatomical characteristics of the teeth scored for 122 specimens of marine reptiles (representing ~50 species) that lived in the Jurassic Sub-Boreal Seaway of the modern-day United Kingdom during the Callovian-Tithonian stages of the Jurassic (Appendix S1). The specimens come from a variety of localities and lithological facies within the Jurassic Sub Boreal Seaway basins[21]. It is possible that the lower number of Oxfordian specimens is related to preservation (or sampling) bias of the Corallian Group facies compared to the fossil-rich and better exposed Oxford Clay Formation and Kimmeridge Clay Formation[21]. However, by focusing on the most commonly collected and preserved fossils (teeth), we minimize these biases. We focused on dental morphology for the following reasons: 1) teeth are more commonly preserved as fossils than any other part of the marine reptile skeleton; 2) teeth were the primary source of information that Massare[7] used to assign marine reptiles into feeding guilds; 3) multivariate analyses of tooth measurements, of the type encapsulated in our dataset, have been commonly applied to other reptile groups (most notably dinosaurs[41,42]) to determine feeding habits and track long-term trends in palaeoecology.

Included in our dataset are teeth belonging to the three major marine reptile clades that lived in the Sub-Boreal Seaway—Plesiosauria, Ichthyosauria, and Thalattosuchia—and

all major subclades within these lineages. We designed our specimen sampling to maximise the number of complete specimens for each taxon in each time bin. We selected an approximately equal number of specimens for each taxon to avoid oversampling biases. All tooth crowns in our dataset are from the anterior part of the tooth row, to avoid inflation of diversity caused by the marked heterodonty of some taxa[15,43,44]. Selecting the largest teeth does not constitute a major problem in the interpretation of the final results because the signal in the analyses is dominated by the discrete characters, which code features that do not significantly change along the tooth row. Additionally, the largest 'fangs' are those that undergo the largest stress during predation, and thus are ideal for investigating feeding ecology[7,43,44]. It is also worth noting that disarticulated teeth cannot always be oriented in their correct mesiodistal orientation, so the distinction between upper or lower jaw teeth is unnecessary.

Each specimen was scored for the 5 continuous and 17 discrete characters in our dataset (Appendix S1), which were selected largely from published phylogenetic and functional datasets[12,18,19,45,46]. The main sources for discrete characters were the analyses of Young et al. (2016)[46], Foffa et al. (2017)[45], and Fischer et al. (2015, 2016, 2017)[12,18,19]; as these studies were designed for specific lineages, it was necessary to modify the definitions and states of some characters, to make them broadly applicable to all marine reptiles. The modified characters were specifically targeted to describe tooth shape, proportions, ornamentation, and cutting edge (carina and denticle) morphologies (Table 1, 2) (Supplementary Figure 1). Most continuous measurements were taken directly from specimens with digital callipers, except for the curvature and crown angles (C4 and C5) that were measured using ImageJ[47], and a small number that were taken from the literature (Supplementary Information, Supplementary Figure 1).

General aspect	**Carinae and serrations**	**Ornamentation**	**Roots**

<table>
<tr><td>C1. Apicobasal crown height – CH</td><td>D1. Crown mediolateral compression</td><td>D2. Carinae: presence or absence</td><td>D7. Enamel surface ornamentation: anastomosed pattern</td><td rowspan="3">D16. Root cross-section</td></tr>
<tr><td>C2. Crown ratio – CR</td><td>D12. Crown cross-section</td><td>D3. Denticles: presence and size</td><td>D8. Enamel ornamentation presence and density: lingual side</td></tr>
<tr><td>C3. Crown base ratio – CBR</td><td>D13. Trifaceted labial side</td><td>D4. ‘Functionally serrated edges’: presence or absence</td><td>D9. Enamel ornamentation presence and density: labial side</td></tr>
<tr><td>C4. Labial-Lingual curvature – LLcufrv</td><td rowspan="3">D15. Tooth crown apex – shape</td><td>D5. Denticles: distribution along the carinae</td><td>D10. Enamel ridges, relief</td><td rowspan="3">D17. Bulbous root larger than the crown</td></tr>
<tr><td rowspan="2">C5. Crown Angle – Cang</td><td>D6. Presence or absence of denticle-like structures</td><td>D14. Enamel texture</td></tr>
<tr><td colspan="2">D11. Ornamentation interfering with the carinae or cutting edges – false denticles</td></tr>
</table>

Table 2. Table of continuous (C) and discrete (D) morphological characters used to represent marine reptile dentitions. See Supplementary Information for extended descriptions of each character.

Multivariate analysis. The continuous characters were standardised using z-transformation (distributions were equalized to the same mean value, $\mu = 0$, and standard deviation, $\sigma = 1$)[11,48]. The entire taxon-character matrix (Appendix S1) was then transformed into a Gower distance matrix (necessary for the combination of ordered discrete and continuous characters)[49] and subjected to Principal Coordinates Analysis (PCO) in PAST v.3 and R v3.4.3[50,51], following the procedure in Stubbs and Benton (2015)[11]. The small number of missing values (8.2% of the total scores) were automatically accounted for by pairwise deletion. The scores of the first three PCO axes (which describe 28.54%, 22.16%, and 12.43% of total variance, respectively: Supplementary Table 1) were used to generate morphospaces for data visualization (Figs. 1-2, Supplementary Figures 1-2), and the 15 PCO axes that accounted for at least 0.5% of total variance were retained for discriminant function analysis, statistical tests of morphospace overlap, and disparity calculations.

We ran a Linear Discriminant Analysis (LDA) (Appendix S3) to test the ability of the

296 PCO scores to assign individuals to the feeding guild assignments of Massare[7]. The 35
297 specimens in our dataset that were also included in Massare's study[7] were a priori assigned to
298 the guilds that Massare originally assigned them to (four guilds total: Pierce [also tested for
299 separate Pierce I and Pierce II], Crunch, Smash, Cut) (for more details see the LDA Guild
300 Sensitivity Analyses in Appendix S4), and the percentages of correct specimen-guild matches
301 were determined using a jackknifing test in PAST v.3[50] (see Supplementary Information,
302 Appendix S3). This revealed that 84% of specimens were correctly assigned to the Massare's
303 original guilds (the same percentage, 84%, if the Pierce I and II guilds of Massare are split
304 into two), indicating a broad correspondence between our quantitative PCO morphospace and
305 Massare's qualitative guilds (see Supplementary Information, Appendix S3, S4).
306 New fossil discoveries and reanalyses of key specimens suggest that some of the guild
307 assignments of Massare may be problematic, perhaps explaining why 16% of specimens are
308 incorrectly assigned by the LDA. Over the last few decades, many specimens used in
309 Massare's study have been re-evaluated (particularly metriorhynchids) and further details of
310 tooth morphology have been described (particularly regarding carinae and denticles)
311 (Appendix S3). Thus, we used the results of our PCO analysis—particularly the visual spread
312 of taxa in morphospace—to modify Massare's guilds into a new system of five guilds: Pierce,
313 Crunch, Smash, Cut, and Generalist (subdivided into Generalist-Pierce, and Generalist-Cut)
314 (Appendix S3, S4). We assigned the same 35 specimens from taxa shared with Massare's
315 study[7] to one of these guilds a priori, and then ran a second LDA, which correctly attributes
316 97.3% of the specimens to the proper guild. This indicates that our morphospace can be used
317 to sensibly cluster species into guilds, and thus be interpreted as a dietary function space.
318 This second LDA also serves to classify each of our 122 specimens into its best-fit guild. The
319 regions of our PCO morphospace occupied by each guild are denoted in Figure 1. This is the
320 first attempt to project Massare's[7] qualitative guilds into a numerically-derived morphospace.

Note that in creating our revised guild system, we preferred a unified Pierce guild over Massare's[7] original subdivision of Pierce I and Pierce II guilds, because this distinction relied on wear patterns and features of cranial morphology that are not captured in our dataset (but see Appendix S4 for sensitivity analyses).

Statistical analyses. Specimens were binned by clade, guild, and time in order to conduct statistical analyses of morphospace overlap and morphological disparity.

We employed a hierarchy of taxonomic bins. We broadly divided the specimens into the three main order-level clades: Plesiosauria, Ichthyosauria, and Thalattosuchia. We then ran additional analyses in which these large clades were subdivided into less inclusive monophyletic groups of family-level, and subfamily-level. Plesiosauria was subdivided into Plesiosauroidea and Pliosauridae. Thalattosuchia was split into Metriorhynchidae and Teleosauridae, both of which were further divided (into Metriorhynchidae/Geosaurinae for the former, and into Machimosaurini/non-Machimosaurini for the latter). As all ichthyosaur specimens belong to Ophthalmosauridae, this group was not subdivided. Finally, for the disparity analyses, we examined three further lineages within Pliosauridae (non-*Pliosaurus* pliosaurids and *Pliosaurus* spp.) and Geosaurinae (the 'T-clade': *Torvoneustes-'Metriorhynchus' hastifer*-Mr. Passmore's specimen clade ; the 'GPD clade': *Plesiosuchus-Dakosaurus-Geosaurus* clade; and 'Basal Geosaurinae', which includes *'Metriorhynchus' brachyrhynchus*, with and without *Tyrannoneustes lythrodectikos* – because of the unstable position of the latter in the latest phylogenetic analyses[17,45]).

We employed four time bins when analysing trends over the Jurassic. These correspond to stage level: Callovian (166.1–163.5 Ma), Oxfordian (163.5–157.3 Ma), Kimmeridgian (157.3–152.1 Ma), and early Tithonian (152.1–148.5 Ma). The average length of these time bins is 4.4 Ma, with a minimum of 2.6 Ma for the Callovian and maximum of 6.2 Ma for the Oxfordian. Given the age uncertainty of several specimens, equal-length bins

were deemed unreasonable because too many specimens would be assigned to multiple time bins, decreasing the power of our analyses. We ran subsidiary analyses in which specimens was also assigned to stratigraphic bins representing the main marine reptile faunas of the Sub-Boreal Jurassic Seaway: Oxford Clay Formation (~Callovian - early Oxfordian), 'Corallian Group' (middle - late Oxfordian), and Kimmeridge Clay Formation (Kimmeridgian - early Tithonian). This binning scheme demonstrates changes in a series of temporally successive Lagerstätten. We recognize that, for both binning schemes, each time bin includes a time-averaged sample, as is necessarily the norm in most palaeoecological analyses of long-term change. Thus, these bins do not exactly represent individual ecosystems that existed at a moment in time, but rather summarize the pool of species present during the finest temporal resolution available.

We assessed whether taxonomic groups significantly overlapped in the overall morphospace, and for each time interval, using non-parametric multivariate analysis of variance (NPMANOVA)[51,11,48] in R[52] (Appendix S2). The null hypothesis is that there is no difference in the location of group centroids in PCO space; significant deviation from the null indicates that the groups in question occupy significantly different areas of morphospace. The p values were adjusted using the false-discovery rate (FDR) method to account for 'false discoveries' error that may be introduced by multiple comparisons[53]. Changes in morphospace occupation over time, if confirmed by NPMANOVA, indicate the migration of clades into different niche space.

We measured the breadth of morphospace occupied by taxa by calculating morphological disparity. We used two metrics to quantify disparity: the sum of variances and the sum of ranges on the PCO axes for each group in question[54]. Variance is a measure of the spread of taxa in morphospace relative to the group centroid, whereas range denotes the overall volume of morphospace occupied by the group. These disparity metrics were

371 calculated in R using functions in the 'dispRity' package[55] Statistical significance of disparity
372 differences between groups, or within groups across time, were assessed by a permutation
373 test developed by Steve Wang[56], which determined whether there was a significant difference
374 in the observed disparity value between the two comparisons and the expected disparity
375 difference between them. As the expected difference is generated based on the size of each
376 group, this procedure accounts for sample size differences between the groups, which
377 otherwise could be a major source of bias (particularly for sum of ranges).
378 We also tracked partial disparity over time, for taxonomic groups and guilds (Fig. 3).
379 The contribution of each group/guild to overall disparity in each time bin was calculated as
380 the average squared distance of each group/guild member point from the overall time bin
381 centroid, with the resulting value weighted by a factor taking into account the sample size of
382 the group/guild compared to the overall sample[57]. This procedure was conducted with the
383 Morphological Disparity Analyses (MDA) package for MATLAB® R2016a v9.0.0[58].

384 **Data availability**

385 The authors declare that all the data supporting the findings of this study are available within
386 the paper and its supplementary information files. The R-codes used to perform statistical
387 tests are available from the corresponding author upon reasonable request.

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Author contributions

DF led the project, conceived the study and wrote the initial draft manuscript. MTY and SLB helped develop the project, edited drafts, and provided guidance on statistical analyses. SLB wrote the final manuscript, which was revised by all authors. DF designed and performed the analyses with technical support from TLS and KGD.

Competing interests

The authors declare no competing interests.

Figure Captions

Figure 1. Morphospace plots showing the distribution of marine reptile specimens based on tooth morphology. **a.** 3D plot of PCO1-PCO2-PCO3, derived from Principal Coordinates Analysis of our dental dataset; **b.** approximate position of the 'feeding guilds' (originally outlined by Massare[7] and modified here) in the PCO morphospace. Tooth drawings depict the general tooth morphologies of key regions of the morphospace.

Figure 2. Morphospace plots showing the distribution of marine reptile clades based on tooth morphology through time, only statistically significant ecological and evolutionary shifts are noted. The morphospaces are 3D plots of PCO1-PCO2-PCO3, derived from Principal Coordinates Analysis (Fig. 1). The radiations and declines of groups through time gradually

592 changed the morphospace/ecosystem composition and partitioning. Note that some groups
593 may have been limited to certain parts of ecomorphospace by evolutionary constraints.
594
595 **Figure 3.** Partial disparity of Jurassic Sub-Boreal Seaway marine reptile, mapped against
596 global sea-level. **a.** Partial disparity of taxonomic groups, **b.** Partial disparity of dietary
597 guilds; **c.** sea-level curve (modified from Haq 1987)[30], with fossil rich-intervals from the Sub-
598 Boreal Seaway noted.